

**Name:** Dr. Harjinder Singh  
**Designation:** Assistant Professor  
**Specialization:** Organic Chemistry  
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### **Education**

**M.Sc. (Hons. School) Chemistry** (2010, Department of Chemistry, Panjab University, Chandigarh)

**NATIONAL ELIGIBILITY TEST (NET)-JRF:-** 2010.

**Ph.D. Organic Chemistry** (5<sup>th</sup> November, 2014, Department of Chemistry, University of Delhi, Delhi).

**Title of Thesis:-** Synthesis of Substituted 1,2,3-Triazoles, their Conjugates and Evaluation of Biological and/or Photophysical Properties.

### **Professional Experience:**

Department of Chemistry, M.M. Modi College, Patiala, India (02 February, 2016 to till date)

Department of Chemistry, SGTB Khalsa College, Delhi University, Delhi (July 2014 to January, 2016)

### **Teaching Interests:**

- General Organic Chemistry
- Stereochemistry
- Spectroscopy
- Reaction Mechanisms

### **Research Interest:**

Computational organic Chemistry, Synthetic Organic Chemistry, Medicinal Chemistry

### **Publications**

1. Jayant Sindhu, **Harjinder Singh**, J.M. Khurana, Chetan Sharma, K.R. Aneja. "Multicomponent synthesis of novel 2-aryl-5-((1-aryl-1H-1,2,3-triazol-4-yl)methylthio)-1,3,4-oxadiazoles using Cu(I) as catalyst and their antimicrobial evaluation". *Aust. J. Chem.*, (2013) **66**: 710 – 717.  
<https://www.publish.csiro.au/ch/ch13082>
2. **Harjinder Singh**, Jayant Sindhu and J.M. Khurana "Efficient, green and regioselective synthesis of 1,4,5-trisubstituted- 1,2,3-triazoles in ionic liquid [bmim]BF<sub>4</sub> and in task-specific basic ionic liquid [bmim]OH", *J. Iran. Chem. Soc.*, (2013) **10**: 883 – 888.

<https://link.springer.com/article/10.1007/s13738-013-0224-6>

3. **Harjinder Singh**, Jayant Sindhu, J.M. Khurana, Chetan Sharma, K.R. Aneja. "A facile eco-friendly one pot five component syntheses of novel 1,2,3-triazole linked penta substituted 1,4-dihydropyridines and their biological and photophysical studies". *Aust. J. Chem.*, (2013) **66**: 1088 – 1096.  
<https://www.publish.csiro.au/ch/CH13217>
4. **Harjinder Singh**, Jayant Sindhu and J.M. Khurana. "Synthesis of biologically as well industrially important 1,4,5-trisubstituted-1,2,3-triazoles using highly efficient, green and recyclable DBU-H<sub>2</sub>O catalytic system". *RSC Adv.*, (2013) **3**: 22360-66.  
<https://pubs.rsc.org/en/content/articlelanding/2013/ra/c3ra44440f/unauth#!divAbstract>
5. Jayant Sindhu, **Harjinder Singh** and J. M. Khurana, "A green, multicomponent, regio- and stereoselective 1,3-dipolar cycloaddition of azides and azomethine ylides generated *in situ* with bifunctional dipolarophiles using PEG-400". *Mol. Diversity*, (2014) **18**,: 345-355.  
<https://link.springer.com/article/10.1007/s11030-014-9505-y>
6. **Harjinder Singh**, Sudesh Kumari and J.M. Khurana "A new green approach the synthesis of 12-aryl-8,9,10,12-tetrahydrobenzo[*a*]xanthene-11-one derivatives using task specific acidic ionic liquid [NMP]H<sub>2</sub>PO<sub>4</sub>," *Chin. Chem. Lett.*, (2014) **25**: 1336-1340.  
<https://www.sciencedirect.com/science/article/abs/pii/S100184171400223X>
7. **Harjinder Singh**, Jayant Sindhu, J.M. Khurana, Chetan Sharma, K.R. Aneja "Efficient one pot synthesis of xanthene-triazole-quinoline/conjugates and evaluation of their antimicrobial activity." *J. Brz. Chem. Soc.*, (2014) **25 (7)**: 1178-1193.  
[http://www.scielo.br/scielo.php?pid=S0103-50532014000700006&script=sci\\_arttext](http://www.scielo.br/scielo.php?pid=S0103-50532014000700006&script=sci_arttext)
8. **Harjinder Singh**, Jayant Sindhu, J.M. Khurana, Chetan Sharma, K.R. Aneja. "Synthesis, biological evaluation and photophysical studies of novel 1,2,3-triazole linked azo dyes." *RSC Adv.*, (2014). **4**: 5915- 26.  
<https://pubs.rsc.org/en/content/articlelanding/2013/ra/c3ra44314k/unauth#!divAbstract>
9. **Harjinder Singh**, Jayant Sindhu, J.M. Khurana, Chetan Sharma, K.R. Aneja "Ultrasound promoted one pot synthesis of novel fluorescent triazolyl spirocyclicoxindoles using DBU based task specific ionic liquids and their antimicrobial activity." *Eur. J. Med. Chem.*, (2014) **77**: 145-54.  
<https://www.sciencedirect.com/science/article/abs/pii/S0223523414002207>
10. **Harjinder Singh**, Jayant Sindhu and J.M. Khurana "Determination of dipole moment, solvatochromic studies and application as turn off-on fluorescence chemosensor of new 3-(4-(dimethylamino)phenyl)-1-(5-methyl-1-(naphthalen-1-yl)-1*H*-1,2,3-triazol-4-yl)prop-2-en-1-one". *Sens Actuators B Chem.*, (2014) **192**: 536– 542.

<https://www.sciencedirect.com/science/article/abs/pii/S0925400513013397>

11. Jayant Sindhu, **Harjinder Singh**, J. M. Khurana, Chetan Sharma and K.R. Aneja “Multicomponent domino process for the synthesis of some novel (Z)-5-(arylidene)-3-((1-aryl-1H-1,2,3-triazol-4-yl)methyl)thiazolidine-2,4-diones using PEG-400 as an efficient and green media and their antimicrobial evaluation,” *Chin. Chem. Lett.*, (2015) 26: 50-54.  
<https://www.sciencedirect.com/science/article/abs/pii/S1001841714003799>
12. Jayant Sindhu, **Harjinder Singh** and J. M. Khurana. “Efficient and green synthesis of spiro[diindenopyridine-indoline]triones using PEG-OSO<sub>3</sub>H-H<sub>2</sub>O and [NMP]H<sub>2</sub>PO<sub>4</sub> under conventional heating and ultrasonic irradiation and their photophysical studies” *Synth. Commun.*, (2015) 45: 202-210.  
<https://www.tandfonline.com/doi/abs/10.1080/00397911.2014.906616>
13. M. Rajeswari, Jayant Sindhu, **Harjinder Singh** and J. M. Khurana,. “An efficient, green synthesis of novel regioselective and stereoselective indan-1,3-dione grafted spirooxindolopyrrolizidine linked 1,2,3-triazoles via a one-pot five-component condensation using PEG-400”. *RSC Adv.*, (2015) 5: 39686-39691.  
<https://pubs.rsc.org/en/content/articlelanding/2015/ra/c5ra03505h/unauth#!divAbstract>
14. **Harjinder Singh**, Jayant Sindhu and J.M. Khurana. “Synthesis, fluorescent properties of xanthene - aminoquinoline derivatives and application as first turn off fluorescent chemosensor for selective and sensitive detection of Th<sup>+4</sup> ions”, *Optical materials*, (2015) 42: 449–457.  
<https://www.sciencedirect.com/science/article/abs/pii/S0925346715000828>
15. **Harjinder Singh**, Jayant Sindhu and J.M. Khurana ”Synthesis, photophysical study of new 7-chloroquinoline based triazolyl chalcones and their derivatives”. *J Lumin.*, (2015) 158: 340-350.  
<https://www.sciencedirect.com/science/article/abs/pii/S0022231314006188>
16. Jayant Sindhu, **Harjinder Singh**, J. M. Khurana, Jitender Kumar Bhardwaj, Priyanka Saraf and Chetan Sharma, “One-pot four component synthesis of functionalized 1H-1,2,3-triazole tethered pyrazolo[3,4-*b*]pyridin-6(7*H*)-ones as novel apoptosis inducers and anti-microbial agents” *Med Chem Res*, (2016) 25: 1813.  
<https://link.springer.com/article/10.1007/s00044-016-1604-0>
17. Sudesh Kumari, **Harjinder Singh**, and J.M. Khurana. “An efficient green approach for the synthesis of novel triazolyl spirocyclic oxindole derivatives via one-pot five component protocol using DBU as catalyst in PEG-400”. *Tetrahedron Letters*. (2016) 57,: 3081–3085.  
<https://www.sciencedirect.com/science/article/pii/S0040403916306177>

18. **Harjinder Singh**, Garima Khanna, Bhaskar Nand and J.M. Khurana. “Metal-free synthesis of 1,2,3-triazoles by azide–aldehyde cycloaddition under ultrasonic irradiation in TSIL [DBU-Bu]OH and in hydrated IL Bu<sub>4</sub>NOH under heating.” *Montash Chem.*, (2016) **147**: 1215-19.  
<https://link.springer.com/article/10.1007/s00706-015-1623-4>
19. **Harjinder Singh**, Garima Khanna and J.M. Khurana. “DBU catalyzed metal free synthesis of fused 1,2,3-triazoles through [3+2] cycloaddition of aryl azides with activated cyclic C-H acids.” *Tetrahedron Letters*. (2016) **57**: 3075–3080  
<https://www.sciencedirect.com/science/article/pii/S0040403916306153>
20. Ashima Singh, **Harjinder Singh**, and J.M. Khurana. “Recyclable Zinc (II) ionic liquid catalyzed synthesis of azides by direct azidation of alcohols using trimethylsilylazide at room temperature.” *Tetrahedron Letters*. (2017) **58 (25)**: 2498-2502.  
<https://www.sciencedirect.com/science/article/pii/S0040403917306275>
21. **Harjinder Singh**, Ashima Singh, and J.M. Khurana “A combined experimental and theoretical approach for structural, spectroscopic, NLO, NBO, thermal and photophysical studies of new fluorescent 5-amino-1-(7-chloroquinolin-4-yl)-1*H*-1,2,3-triazole-4-carbonitrile using density functional theory.” *Journal of Molecular Structure*, (2017) **1147**: 725-734.  
<https://www.sciencedirect.com/science/article/abs/pii/S0022286017309316>
22. **Harjinder Singh**, M. Rajeshwari, and J.M. Khurana. “Synthesis, photophysical studies, and application of novel 2,7-bis(1-butyl-1*H*-1,2,3-triazol-4-yl)methoxy)naphthalene as a highly selective, reversible fluorescence chemosensor for detection Fe<sup>3+</sup> ions”. *Journal of Photochemistry and Photobiology- A: Chemistry*. (2018) **(353)** : 424–432.  
<https://www.sciencedirect.com/science/article/abs/pii/S1010603017314302>
23. **Harjinder Singh**. “The mechanistic study of reaction between N-benzoyl carbamates and aliphatic/aromatic amines for synthesis of substituted N-benzoyl urea derivatives: A DFT approach”. *Structural Chemistry*. (2019) **30 (1)**: 37-51  
<https://link.springer.com/article/10.1007/s11224-018-1171-8>
24. Ashima Singh, **Harjinder Singh**, and J.M. Khurana “Computational study of new 1,2,3-triazole derivative of lithocholic acid: structural aspects, non-linear optical properties and molecular docking studies as potential PTP 1B enzyme inhibitor” *Computational Biology and Chemistry*. (2019). **78**:144-52.  
<https://www.sciencedirect.com/science/article/abs/pii/S1476927118305188>

25. **Harjinder Singh**. “A DFT approach for theoretical and experimental study of structure, electronic, Hirshfeld surface and spectroscopic properties of 2- of 12-(4-bromophenyl)-2-(prop-2-ynoxy)-9,10-dihydro-8H-benzo[a]xanthen-11(12H)-on single crystal” *Chemical Physics*. (2019) **524 (1)**: 1-13.  
<https://www.sciencedirect.com/science/article/abs/pii/S0301010418313636>
26. **Harjinder Singh**. “A DFT investigation on aromatic nucleophilic substitution (SN Ar) reaction between 4-fluoro-1-naphthaldehyde/4-fluoro-2-naphthaldehyde/1-fluoro-2-naphthaldehyde/1-fluoronaphthalene and methylthiolate ion in gas phase and in protic/aprotic solvents” *Structural Chemistry*. (2020) **31**: 2205-2213.  
<https://doi.org/10.1007/s11224-020-01581-1>
27. **Harjinder Singh**. “Crystal structure, surface analysis, and computational investigations of 1-(4-chloro-3-nitrophenyl)-6,7-dihydro-1H-benzo[d][1,2,3]triazol-4(5H)-one as potential acceptor molecule for photovoltaics applications” *Journal of Molecular Structure*, (2022) **1254**: 132349.  
<https://www.sciencedirect.com/science/article/abs/pii/S0022286022000229>
28. **Harjinder Singh**, V Saini, “Development, Synthesis, Computational and in silico investigations of Pd (II)-Catalyzed Aryl Fluorinated and Hydroxylated Sulfonamides” *Journal of Molecular Structure*, (2022) **1266**: 133481.  
<https://www.sciencedirect.com/science/article/abs/pii/S0022286022011371>
29. Nishita Chauhan, **Harjinder Singh**, Kamal Nain Singh, Jeffrey M McKenna, Vaneeet Saini, “Development, Synthesis, and in silico Investigations of Novel Acyclic Allyl Fluoride Derivatives” *Synthesis*, (2022) **55 (05)**: 837-845.  
<https://www.thieme-connect.com/products/ejournals/abstract/10.1055/a-1961-8013>
30. **Harjinder Singh**, A DFT insight into structure, NBO, NCI, QTAIM, vibrational, and NLO properties of cationic amino acid ionic liquid [Pro-H]<sup>+</sup>BF<sub>4</sub><sup>-</sup> *Structural Chemistry*, (2023) 1-13  
<https://link.springer.com/article/10.1007/s11224-023-02195-z>
31. **Harjinder Singh**, A mechanistic investigation of metal-free allylic fluorination of styrenes for the synthesis of allyl fluoride derivatives using density functional theory, *Structural Chemistry*, (2023) 1-9.  
<https://link.springer.com/article/10.1007/s11224-023-02253-6>

## Conference / Seminars

### A) Paper presented:

1. **Harjinder Singh** and J.M. Khurana (2012) Synthesis of Substituted 1,2,3-Triazoles in Ionic Liquids [bmim]BF<sub>4</sub> and [bmim]OH” in the National Conference on New Frontier in Chemistry, held at Department of Chemistry, Kurukshetra University, Kurukshetra, India.

2. **Harjinder Singh** and J.M. Khurana (2012) 14<sup>th</sup> National Symposium in Chemistry (NSC-14) and 6<sup>th</sup> CRSI – RSC Symposium in Chemistry at National institute for interdisciplinary science and technology, Thiruvananthapuram, India
3. **Harjinder Singh** and J.M. Khurana (2014) “Novel Green Approaches for Efficient
4. Synthesis of Trisubstituted Triazoles” at 16<sup>th</sup> CRSI National Symposium in Chemistry held at IIT Bombay, India.
5. **Harjinder Singh** (2018) “Recyclable Zinc based ionic liquid catalyzed synthesis of azides at room temperature” at UGC sponsored 9<sup>th</sup> National Conference on Recent Advances in Chemical, Biological and Environmental Sciences held at M M Modi College, Patiala, India.
6. **Harjinder Singh** (2019) “The mechanistic study of reaction between N-benzoyl carbamates and aliphatic/aromatic amines for synthesis of substituted N-benzoyl urea derivatives: A DFT approach” at UGC sponsored 10<sup>th</sup> National Conference on Recent Advances in Chemical, Biological and Environmental Sciences held at M M Modi College, Patiala, , India on 12<sup>th</sup> -13<sup>th</sup> April 2019.
7. **Harjinder Singh** (2022) ”A DFT investigation on aromatic nucleophilic substitution (S<sub>N</sub>Ar) reaction between 4-fluoro-1-naphthaldehyde/4-fluoro-2-naphthaldehyde/1-fluoro-2-naphthaldehyde/1-fluoronaphthalene and methylthiolate ion in gas phase and in protic/aprotic solvents” at UGC sponsored 11<sup>th</sup> National Conference on Recent Advances in Chemical, Biological and Environmental Sciences held at M M Modi College, Patiala, , India on 11<sup>th</sup> -12<sup>th</sup> April 2023.

## **B) Attended**

1. RC Paul Symposium in Chemistry 11<sup>th</sup> -14<sup>th</sup> Feb, 2011 at Department of Chemistry, Panjab University, Chandigarh.
2. 4<sup>th</sup> Science conclave:-A Congregation of Nobel laureates and eminent scientists organized at IIIT-A, Allahabad, 26<sup>th</sup> Nov-2<sup>nd</sup> Dec, 2011.
3. Training workshop on Green chemistry for tomorrow’s world organized by Royal Chemical Society (north India section), 26<sup>th</sup> Dec, 2011 at University Guest House, University of Delhi, Delhi.
4. 4<sup>th</sup> Workshop on Bioinformatics and Molecular Modeling in Drug Design, held at Dr. B.R. Ambedkar Center for Biomedical Research (ACBR), University of Delhi during 18<sup>th</sup> -20<sup>th</sup> Jan, 2012.
5. 5<sup>th</sup> National Seminar in New Frontier in Chemistry, held at Punjabi University, Patiala, 15<sup>th</sup> -16<sup>th</sup> Feb 2013.

6. 20<sup>th</sup> ISCB International Conference on “Chemistry and Medicinal Plants in Translational Medicine for Healthcare” held at Department of Chemistry, University of Delhi, Delhi on 1<sup>st</sup> -4<sup>th</sup> March 2014.

### **Workshops and training courses**

1. Attended UGC sponsored Seven Day Faculty Development Program on the theme of “Academic Writing From Critical Appreciation to Publication” held M M Modi College, Patiala from January 9-16, 2017.
2. Attended Seven Day Faculty Development Program on the theme of “Contemporary issues in Higher Education” held M M Modi College, Patiala from July 20-26, 2018.
3. Attended Faculty Development Program on the theme of “Emerging issues and challenges in Higher Education” held M M Modi College, Patiala from July 17<sup>th</sup> -22, 2019.
4. 4-Week induction/orientation programme for faculty in University/colleges/HEI from June 26-July 24, 2020, held at teaching learning centre Ramanujan College, University of Delhi, Delhi.
5. 7-Day virtual national level capacity building program on integration of pedagogy and technology from 13<sup>th</sup> July– 19<sup>th</sup> July 2021 organised by IQAC, M M Modi College, Patiala.
6. 89<sup>th</sup> Refresher Course in Chemistry from 29<sup>th</sup> November-11<sup>th</sup> December 2021, organised by UGC-HRDC, Punjabi University, Patiala.
7. FDP on Research Methodology from 12<sup>th</sup> January to 19<sup>th</sup> January 2022, organised by IQAC, M M Modi College, Patiala.
8. Symposium, on NEP-2020-Policy Praxis organized by IQAC, M M Modi College, Patiala on 8<sup>th</sup> May 2023.
9. NEP 2020 Orientation and Sensitization programme under “Malaviya Mission Teacher Training Programme” of UGC organized by Punjabi University, Patiala from 5<sup>th</sup> -14<sup>th</sup> Feb 2024.

